

# Multiple mass solvers

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We present a general method to construct multiple mass solvers from standard algorithms. As an example, the BiCGstab-M algorithm is derived.

## 1. INTRODUCTION

It has been discussed recently that, using Krylov space solvers, the solutions of shifted linear equations, where  $(A + \sigma)x - b = 0$  has to be calculated for a whole set of values of  $\sigma$ , can be found at the cost of only one inversion. This kind of problem arises in quark propagator calculations for QCD as well as other parts of computational physics (see [1]). It has been realized that several algorithms allow to perform this task using only as many matrix-vector operations as the solution of the most difficult single system requires. This has been achieved for the QMR [1], the MR [2] and the Lanczos-implementation of the BiCG method [3]. We present here a unifying discussion of the principles to construct such algorithms and succeed in constructing shifted versions of the CG, CR, BiCG and BiCGstab algorithms [4], using only two additional vectors for each mass value.

## 2. METHOD

The iterates of Krylov space methods, especially the residuals  $r_n$ , are generally polynomials  $P_n(A)$  of the matrix applied to some initial vector  $r_0$ . The polynomial generating the residual generally has to be an approximation to zero in some region enclosing the spectrum of  $A$  while satisfying  $P_n(0) = 1$ . The key to the method is the observation that shifted polynomials, defined by

$$P_n^\sigma(A + \sigma) = c_n^\sigma P_n(A), \quad (1)$$

are useful objects, since vectors generated by these shifted polynomials can be calculated for

multiple  $\sigma$  values using no additional matrix-vector multiplications. We expect  $c_n^\sigma < 1$  if the condition number of  $A + \sigma$  is smaller than the one of  $A$ , which is confirmed in numerical tests.

Generally the polynomial generated in a solver is defined by some recursion relation. We will therefore need to know the recursion relation for the shifted polynomial, too, which can be found easily by parameter matching. Here, we discuss only polynomials which satisfy  $P(0) = 1$ , but more general normalisation conditions are handled analogously. For the two-term recursion relation

$$P_{n+1}(x) = (\alpha_n x + 1)P_n(x) \quad (2)$$

we find for the polynomial shifted by  $\sigma$

$$P_{n+1}^\sigma(x) = \left( \frac{\alpha_n}{1 - \sigma\alpha_n} x + 1 \right) P_n^\sigma(x) \quad (3)$$

$$= \left( \prod_i \frac{1}{1 - \sigma\alpha_i} \right) P_{n+1}(x - \sigma). \quad (4)$$

This formula has also been found in [2] with different methods. From (3) we can read off the parameters of the shifted polynomial, while (4) determines  $c_n^\sigma$ . Note that this formula holds for any choice of  $\alpha_n$ . We can easily generalize this method to three-term recurrences

$$P_{n+1}(x) = (\alpha_n x + \beta_n)P_n(x) + \gamma_n P_{n-1}(x) \quad (5)$$

and find explicit expressions for the parameters of the shifted polynomial. It turns out that the Lanczos polynomials for the matrices  $A$  and  $A + \sigma$  fulfill (1) automatically (this was the original observation in [1]). We derived the shifted polynomial however for arbitrary choices of parameters

$\alpha$  and  $\beta$ . The most interesting case are coupled two-term recurrences, since they have superior stability properties over three-term recurrences. We consider the general recurrence

$$Q_n(x) = P_n(x) + \alpha_n Q_{n-1}(x) \quad (6)$$

$$P_{n+1}(x) = P_n(x) + \beta_n x Q_n(x). \quad (7)$$

In  $CG$ -type algorithms, the parameters are chosen so that  $P_n(x)$  is the Lanczos-polynomial (normalized to  $P(0) = 1$ ). We thus demand  $P_n^\sigma(x + \sigma) = c_n^\sigma P_n(x)$ . By transforming the above relation to a simple three-term recurrence and applying the formulae found in this case for the shifted parameters we find

$$c_{n+1}^\sigma = \frac{c_n^\sigma}{\frac{\beta_n}{\beta_{n-1}} \alpha_n \left(1 - \frac{c_n^\sigma}{c_{n-1}^\sigma}\right) + (1 - \sigma \beta_n)} \quad (8)$$

$$\beta_n^\sigma = \beta_n \frac{c_{n+1}^\sigma}{c_n^\sigma} \quad (9)$$

$$\alpha_n^\sigma = \alpha_n \frac{c_n^\sigma \beta_{n-1}^\sigma}{c_{n-1}^\sigma \beta_{n-1}}. \quad (10)$$

It can easily be checked that  $Q_n^\sigma(x + \sigma) \neq c_n^\sigma Q_n(x)$ , so if we want to use this recursion relation in an algorithm we have to replace

$$\beta_n^\sigma(x + \sigma) Q_n^\sigma(x) = c_{n+1}^\sigma P_{n+1}(x) - c_n^\sigma P_n(x) \quad (11)$$

in the shifted systems. Since in  $CG$ -type algorithms the update of the solution vector involves  $Q_n(x)v_0$ , this vector has to be iterated and stored for all shifted systems.

### 3. APPLICATIONS

Using the above formulae, we can easily derive a variety of linear system solvers as shown in table 1. We present here only the algorithm of greatest interest for quark propagator calculations, BiCGstab-M.

#### 3.1. BiCGstab-M

The BiCGstab-M algorithm is a mixture between the BiCG and the MR algorithm. It is therefore not surprising that we can simply use the formulae for the two-term and the coupled two-term recurrences and construct a shifted algorithm. In the BiCGstab algorithm [5], we gen-

Method	Reference	Memory
MR-M	[2,4]	$N$
CR-M	[4]	$2N$
QMR-M (3-term)	[1]	$3N$
QMR-M (2-term)	[6,4]	$3N$
TFQMR-M	[1]	$5N$
BIORESU	[3,4]	$2N$
BiCG-M	[4]	$2N$
BiCGstab-M	[4]	$2N + 1$

Table 1

Memory requirements and references for shifted system algorithms for unsymmetric or nonhermitean matrices. We list the number of additional vectors necessary for  $N$  additional values of  $\sigma$  (which is independent of the use of the  $\gamma_5$ -symmetry).

erate the following sequences

$$r_n = P_n(A)R_n(A)r_0 \quad (12)$$

$$w_n = P_n(A)R_{n-1}(A)r_0 \quad (13)$$

$$s_n = Q_n(A)R_n(A)r_0 \quad (14)$$

where  $Z_n(x)$  and  $Q_n(x)$  are exactly the BiCG-polynomials and  $R_n(x)$  is derived from a minimal residual condition. For the shifted algorithm we demand

$$P_n^\sigma(x + \sigma) = c_n^\sigma P_n(x), \quad R_n^\sigma(x + \sigma) = d_n^\sigma R_n(x). \quad (15)$$

Using the above formulae we can explicitly determine the constants  $c$  and  $d$  and the shifted parameters of the polynomials. The remaining difficulty is to derive the iteration for the solution  $x_n$  and the vector  $s_n$ . The update of these two vectors has the form

$$x_{n+1} = x_n - \beta_n s_n + \chi_n w_{n+1} \quad (16)$$

$$s_{n+1} = r_{n+1} + \alpha_{n+1}(s_n - \chi_n A s_n) \quad (17)$$

This means we have to eliminate  $A s_n$  from the update of  $s_n$ . The updates for the shifted vectors  $x_n^\sigma$  and  $s_n^\sigma$  then look as follows:

$$x_{n+1}^\sigma = x_n^\sigma - \beta_n^\sigma s_n^\sigma + \chi_n^\sigma c_n^\sigma d_{n-1}^\sigma w_{n+1} \quad (18)$$

$$s_{n+1}^\sigma = c_{n+1}^\sigma d_{n+1}^\sigma r_{n+1} + \alpha_{n+1}^\sigma \times \left( s_n^\sigma - \frac{\chi_n^\sigma}{\beta_n^\sigma} (c_{n+1}^\sigma d_n^\sigma w_{n+1} - c_n^\sigma d_n^\sigma r_n) \right) \quad (19)$$

We therefore need to introduce 2 vectors for each shifted system and one additional vector to store  $r_n$ . Note that the case  $\beta_n = 0$  leads to a breakdown of the BiCGstab algorithm and does not introduce any new problems for the shifted method.

The convergence of the shifted algorithms can be verified by checking that  $c_n r_n \leq 1$ . It is however generally advisable for all shifted algorithms to test all systems for convergence after the algorithm finishes since a loss of the conditions (15) due to roundoff errors might lead to erratic convergence.

#### 4. LIMITATIONS

The most serious limitation of the method is given by the fact that the starting residual for all systems must be the same, which excludes  $\sigma$ -dependent left preconditioning. Furthermore, preconditioning must retain the shifted structure of the matrix. This means that especially even-odd preconditioning is not applicable. To stabilize the algorithm, however, one can apply polynomial preconditioning:

$$P(A)Ay = b, \quad x = P(A)y. \quad (20)$$

We must have

$$P^\sigma(A + \sigma)(A + \sigma) = P(A)A + \eta. \quad (21)$$

Note that  $P^\sigma$  might not be a good preconditioner for  $A + \sigma$ , which is compensated for by the faster convergence of the shifted system. A linear preconditioner, which was also proposed in [2], is given by

$$P^\sigma(x) = 2(\sigma + m) - x. \quad (22)$$

For the Wilson and clover matrix, this polynomial has the property that  $P^\sigma(x)$  is a good preconditioner for  $A + \sigma$ . This preconditioner has been found to work well in those cases. Higher order polynomials can be derived from condition (21).

#### 5. CONCLUSIONS

We presented a simple point of view to understand the structure of Krylov space algorithms for shifted systems, allowing us to construct shifted versions of most short recurrence Krylov space

algorithms. The shifted CG-M and CR-M algorithm can be applied to staggered fermion calculations. Since efficient preconditioners for the staggered fermion matrix are not known, a very large improvement by these algorithms can be expected. We presented the BiCGstab-M method, which, among the shifted algorithms, is the method of choice for quark propagator calculations using Wilson (and presumably also clover) fermions if enough memory is available. The numerical stability of the algorithms has been found to be good [4]. Roundoff errors might however in some cases affect the convergence of the shifted systems so that the final residuals have to be checked. Other discussions can be found in [7,8].

#### Acknowledgements

This work was supported in part by the U.S. Department of Energy under Grant No. DE-FG02-91ER40661. I would like to thank S. Pickels, C. McNeile and S. Gottlieb for helpful discussions.

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